



# Numerical Simulations For CO<sub>2</sub> Storage in Saline Aquifer

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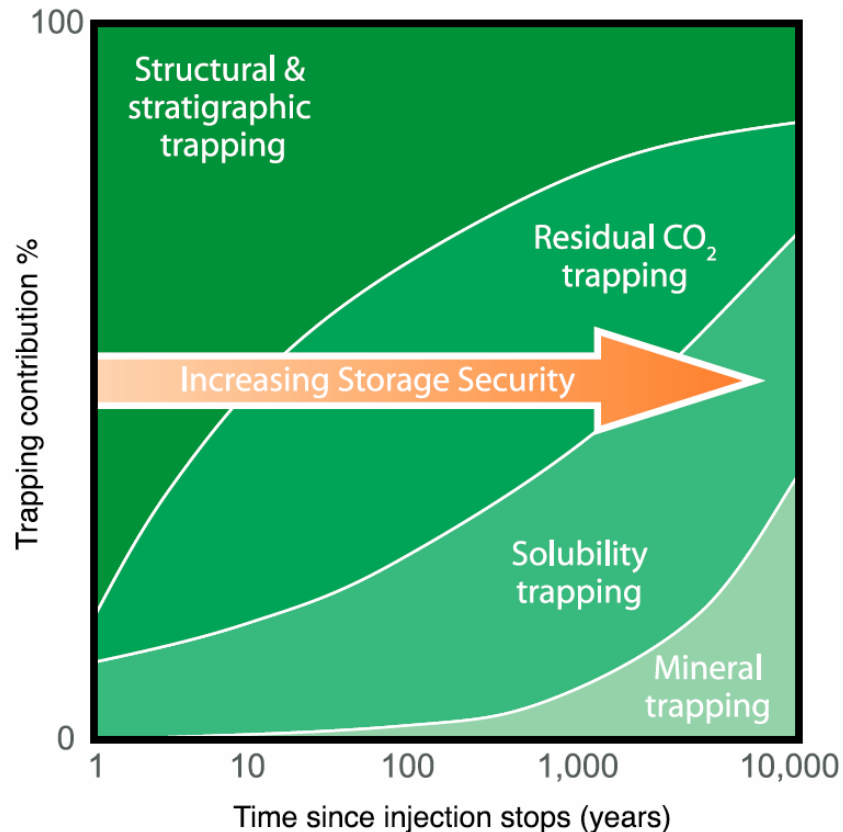


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# Long-Term Fate of Stored CO<sub>2</sub>



## Different Storage Modes

1. free gas
2. trapped gas
3. dissolved in brine
4. sequestered as solid minerals

1, 2, and 3 can be simulated with multiphase flow simulator; 4 can be simulated by reactive transport model.

Source: 2005 IPCC Special Report on Carbon Dioxide Capture and Storage;  
<http://www.ipcc.ch/activity/srccs/index.htm>

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# The simulation technology needed to solve these problems(1)

- ✓ How do the relative proportions of  $\text{CO}_2$  in these different storage modes change over time?
- ✓ How does the evolution of  $\text{CO}_2$  leaks depend on coupling of chemical, mechanical, and thermal effects? What is the fate of leaking?
- ✓ What fraction of subsurface volume can be accessed by  $\text{CO}_2$  ?
- ✓ How is the utilization of subsurface space affected by viscous instability, gravity override and formation heterogeneities?



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# The simulation technology needed to solve these problems(2)

- ✓ Can CO<sub>2</sub> leaks self-seal or self-enhance?
- ✓ What is the role of relative permeability and capillary pressure effects in CO<sub>2</sub> containment and leakage?
- ✓ What is the role of different phase compositions and phase changes in CO<sub>2</sub> leakage?(supercritical, liquid ,gaseous CO<sub>2</sub> , dissolved in water)?
- ✓ What is the pressure build up and CO<sub>2</sub> plume distribution after CO<sub>2</sub> injection?
- ✓ Help for design and analysis of tests.

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# Simulators for CO<sub>2</sub> Storage in Saline Aquifers

- ECLIPSE
- FEHM
- GEM
- GPRS
- TOUGH2
- STOMP
- Other simulators : COORES, DuMu, IPARS-CO2, MUETE, RockFlow, RTAFF2



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# TOUGH Family Code For CO<sub>2</sub> Sequestration

## Fluid dynamics: TOUGH2/ECO2N

- Multiphase flows of water/CO<sub>2</sub>/NaCl mixtures
- Applications to studies of reservoir dynamics, storage capacity, CO<sub>2</sub> leakage

## Geochemistry: TOUGHREACT/ECO2N

- Reactions between gas-aqueous-solid phases
- Study mineral trapping, caprock integrity, natural CO<sub>2</sub> reservoirs

## Geomechanics: TOUGH-FLAC

- TOUGH2 coupled to commercial FLAC3D geomechanics code
- Stress-strain: analyze leakage through caprock and faults

## Large Scale Simulations: TOUGH2-MP/ECO2N



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# Computation Challenging

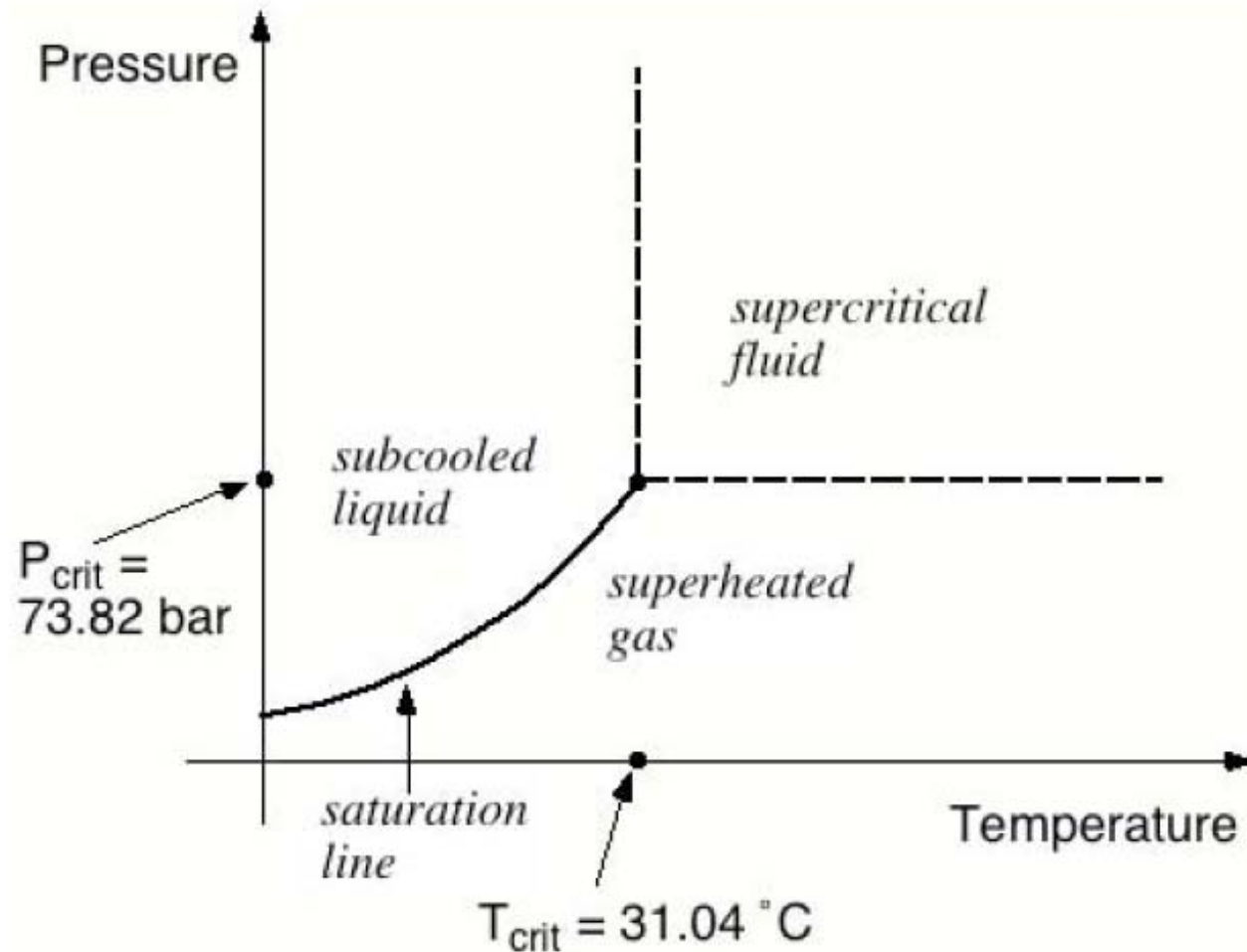
- ✓ Site characterization needs basin-scale model
- ✓ Refined grids are needed for catching CO<sub>2</sub> convection
- ✓ Multi-Scale, multiphase flow
- ✓ Complex geochemical reaction and mechanical processes
- ✓ Leakage of CO<sub>2</sub> through boreholes, faults, and other high permeability paths (may be non-Darcy flow)
- ✓ THMC coupling simulations



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# Phase Diagram of CO<sub>2</sub> for Numerical Simulations



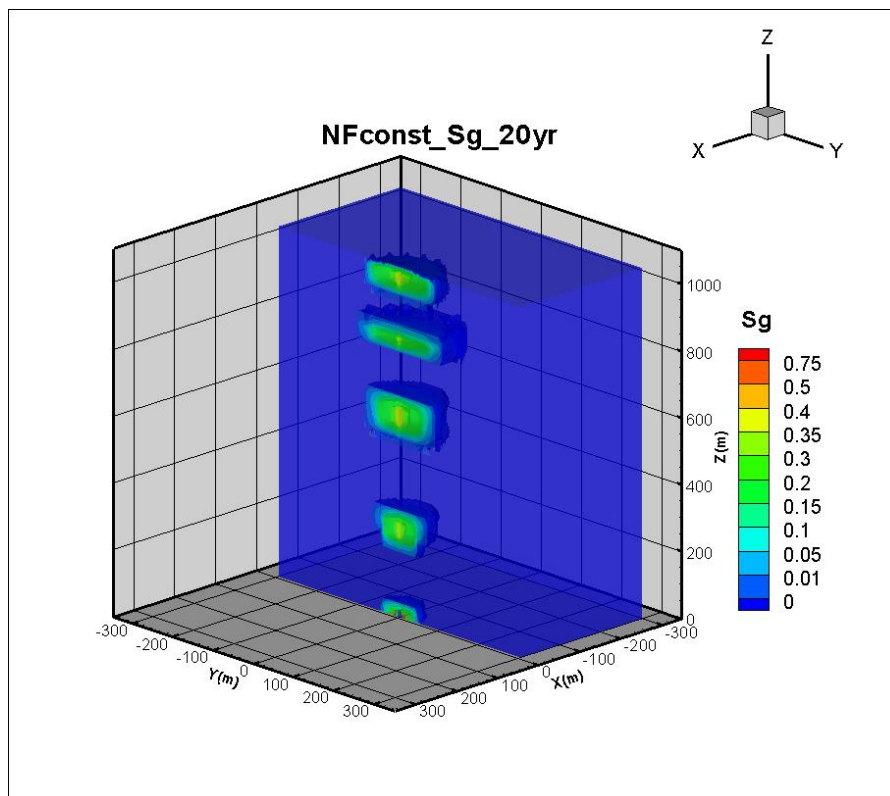
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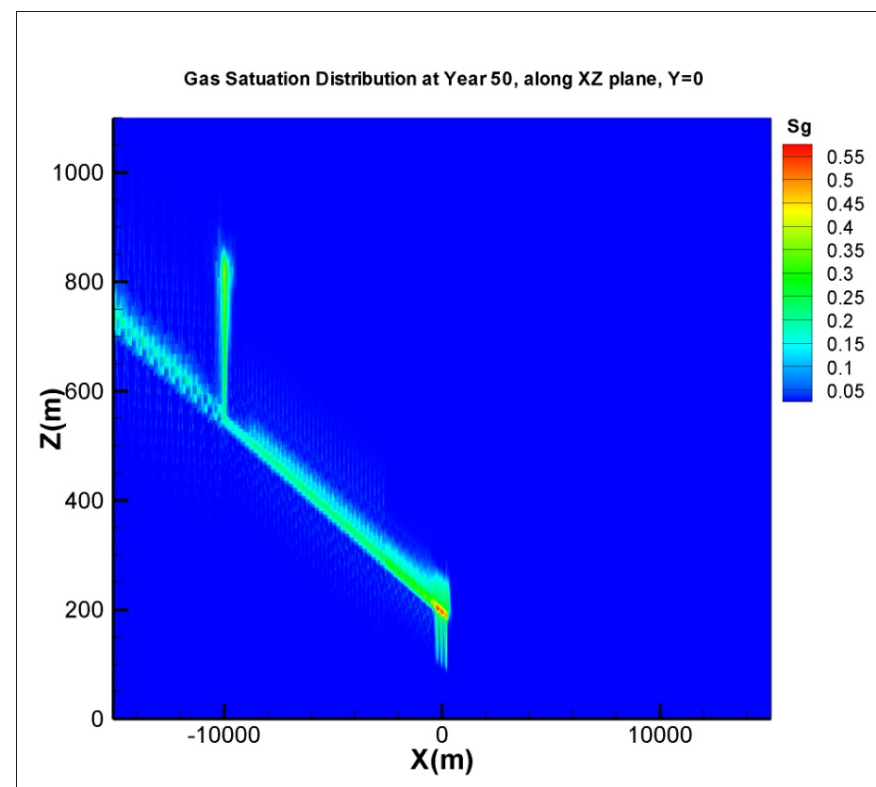
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# Examples for permeability influences on CO<sub>2</sub> storage



Simulation results for a storage site in Western China



Simulation results for a storage site in Eastern China

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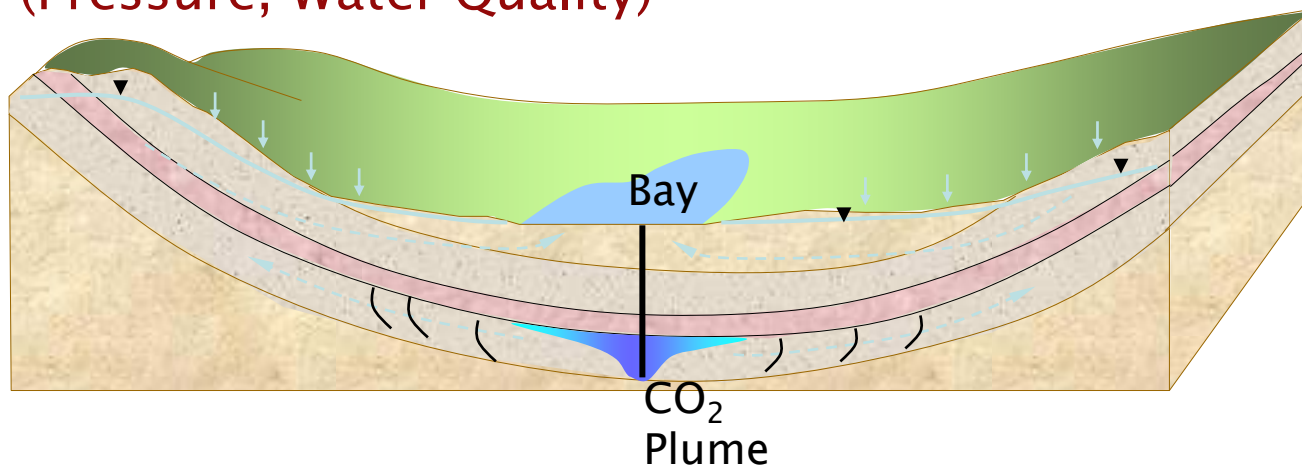
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# Example 1: Tokyo Bay Model

(from Hajime, Zhang et al. 2008)

- Large-scale injection (several  $\text{MtCO}_2/\text{yr}$ ) into virgin aquifers would:
  - Push large volume of water out of the aquifers.
  - Potentially affect subsurface groundwater environment (Pressure, Water Quality)



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# Lithofacies Analysis

| Age        |             | Ma             | Group/Formation |                                 |          | Thickness Ratio | Lithofacies West/East |       |          |       |
|------------|-------------|----------------|-----------------|---------------------------------|----------|-----------------|-----------------------|-------|----------|-------|
| Quaternary | Holocene    |                | 0.6             | fluvial/river terrace sediments |          |                 | —                     | —     |          |       |
|            | Pleistocene | Late           |                 | Shimosa Group                   |          |                 | —                     | —     |          |       |
|            |             | Middle         |                 | Kazusa Group                    | Upper    | Kongochi        |                       | 35%   | sandy    |       |
|            |             |                |                 |                                 |          | Upper Kasamori  |                       |       | muddy    | sandy |
|            |             |                |                 |                                 |          | Lower Kasamori  |                       |       | gravelly |       |
|            |             |                |                 |                                 |          | Chonan          |                       | 20%   | sandy    |       |
|            | Ichijiyuku  |                |                 |                                 |          | 5%              | gravelly              | sandy |          |       |
|            | Early       | Kokumoto       |                 | 15%                             | muddy    |                 |                       |       |          |       |
|            |             | Umegase        |                 | 25%                             | sandy    |                 |                       |       |          |       |
|            |             | Higashi Higasa |                 |                                 | gravelly |                 |                       |       |          |       |
|            |             | Otadai         |                 |                                 | 20%      | muddy           |                       |       |          |       |
|            |             | Kiwada         |                 | 10%                             |          |                 |                       |       |          |       |
| Tomiya     | Tomiya      | 20%            | muddy           |                                 |          |                 |                       |       |          |       |
|            | Ohara       |                |                 |                                 |          |                 |                       |       |          |       |
|            | Namihana    | 20%            |                 |                                 |          |                 |                       |       |          |       |
|            | Katsuura    | 30%            |                 |                                 | gravelly |                 |                       |       |          |       |
| Kurotaki   |             |                |                 |                                 |          |                 |                       |       |          |       |
| Neocene    | Pleistocene |                | Awa Group       |                                 |          | —               | —                     | —     |          |       |
|            | Miocene     |                |                 |                                 |          |                 |                       |       |          |       |

# Model

|                       |      |
|-----------------------|------|
| fluvial/river terrace | Sand |
| Shimosa               | Mud  |
| Upper Kazusa          | Sand |
| Middle Kazusa         | Mud  |
|                       | Sand |
| Lower Kazusa          | Mud  |
|                       | Sand |
|                       | —    |

Simplified

Shallow Seal layer

Deep Seal layer

Storage Aquifer

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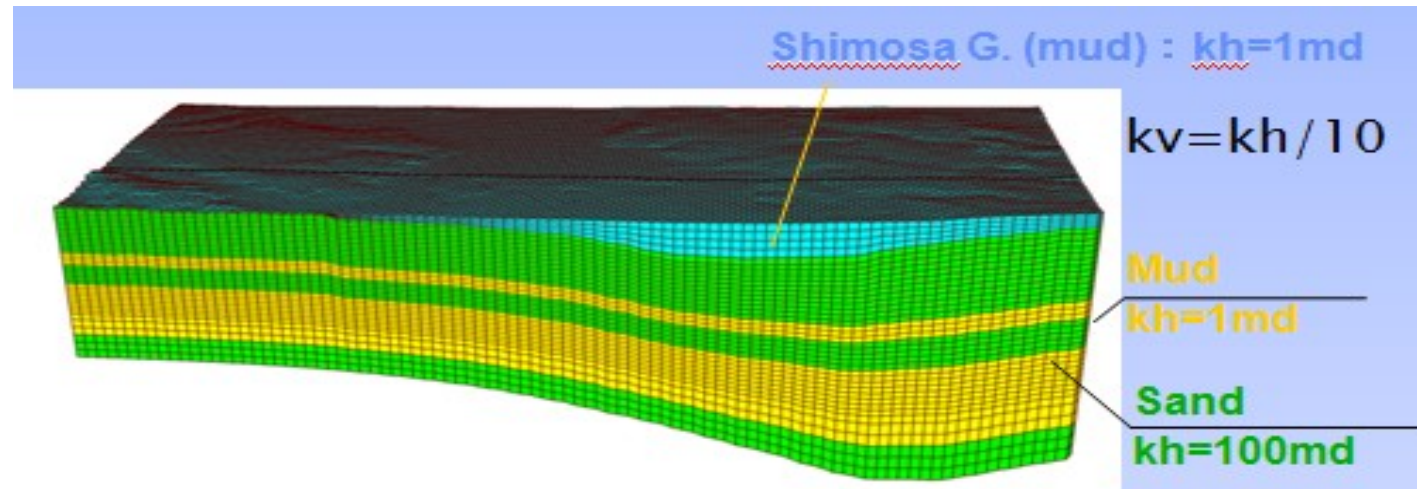
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# Hydrogeological Model(1)

## Continuous Layer Model

Assume perfect lateral continuity



|           |                      |                |
|-----------|----------------------|----------------|
| Base Case | Rock compressibility | $10^{-9}$ 1/Pa |
|           | Porosity             | 40%            |

Sensitivity cases

1. Rock compressibility  $10^{-9} \rightarrow 10^{-8}$  1/Pa
2. Permeability of mud layers  $1 \rightarrow 10$  md

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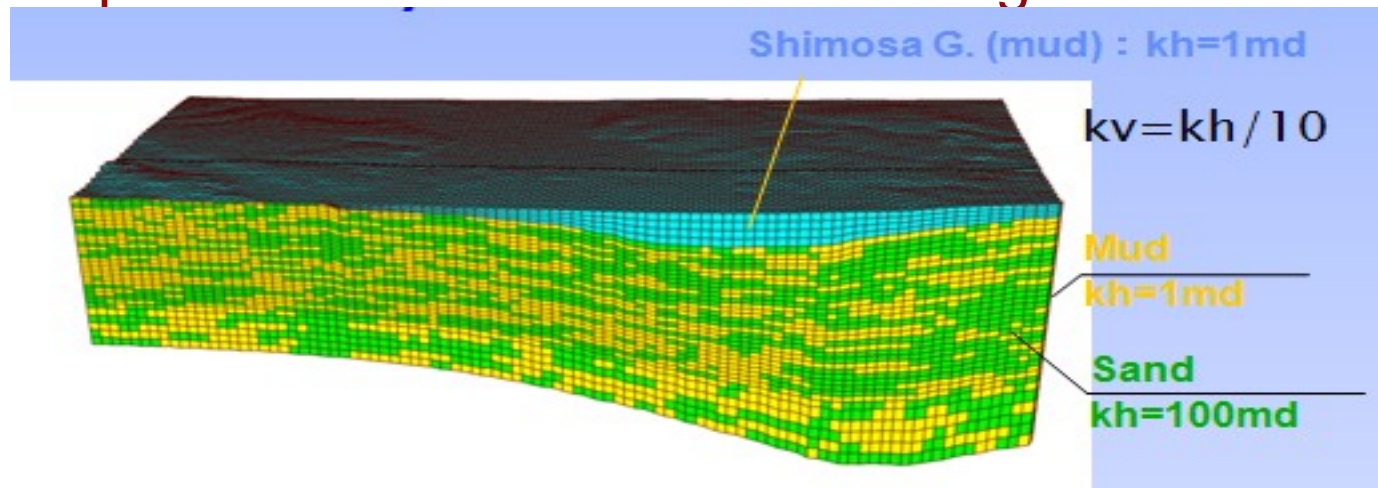
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# Hydrogeological Model(2)

## Discontinuous Layer Model

Represents lateral lithofacies changes



### ➤ Geostatistical Unconditional Simulation(10 realizations)

- Lateral lithofacies changes
- Continuity of layers

5km (horizontal)

20m (vertical)

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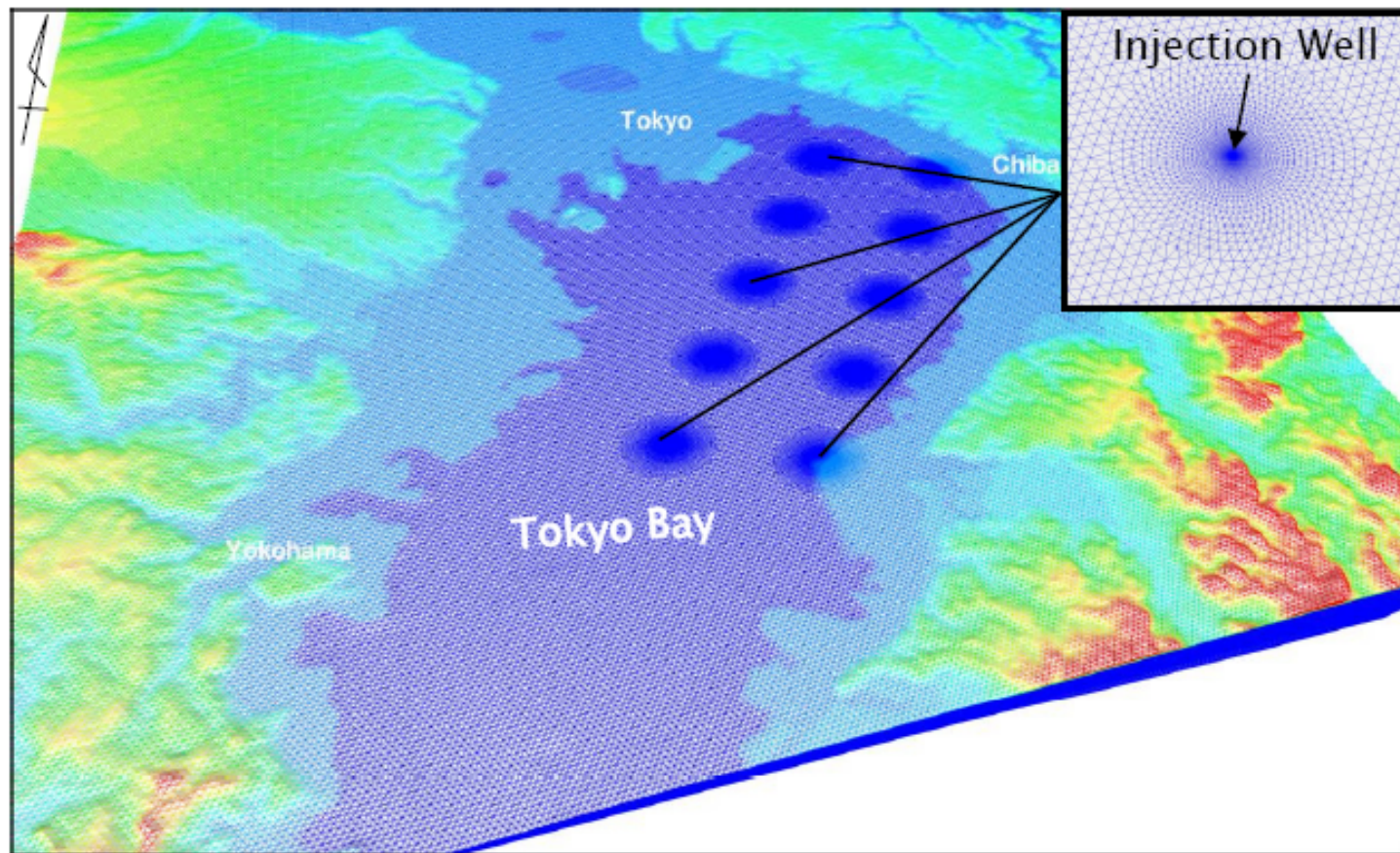


Figure 1. 3D grid system (about 10 million gridblocks, only connections are shown)

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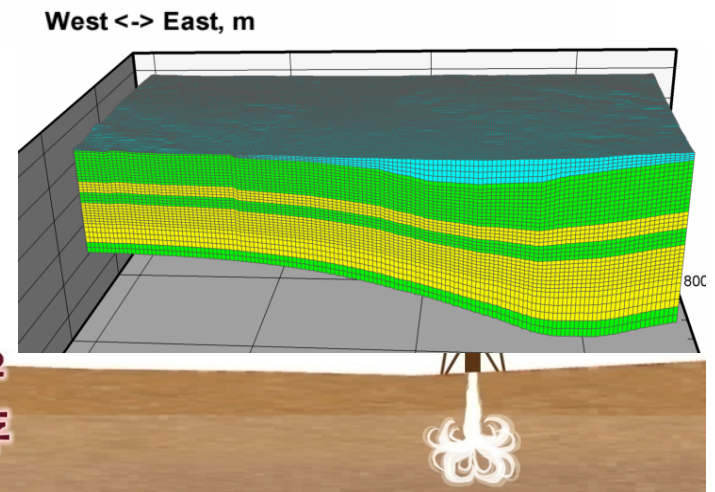
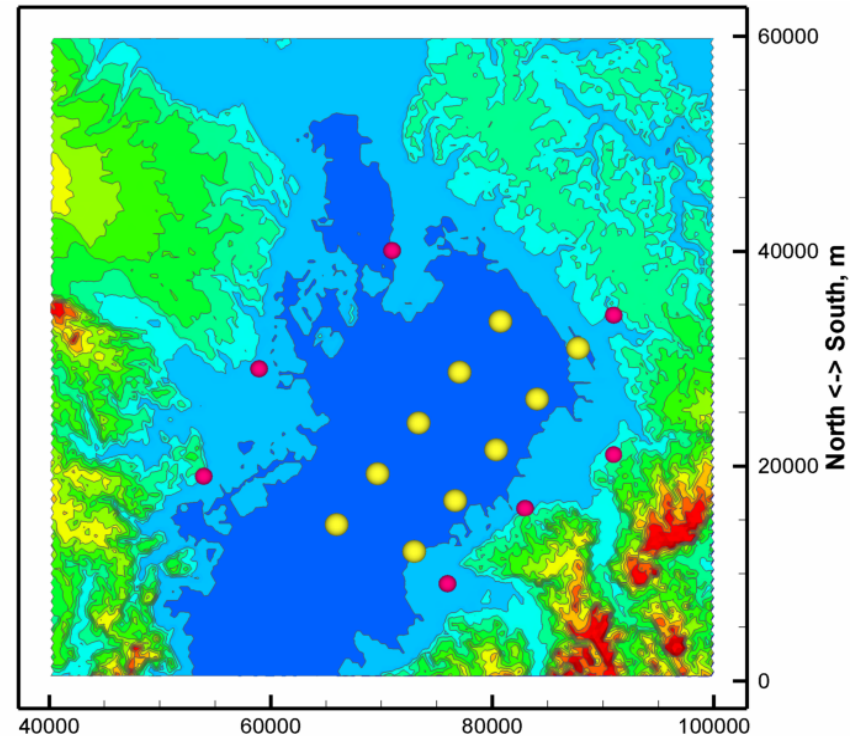
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# Hypothetical CO<sub>2</sub> Injection

- Target aquifer:
  - Middle Kazusa Group
  - Depth = 800 to 1000m
- Supercritical CO<sub>2</sub>  
e.g., Density  $\sim 0.56 \text{ t/m}^3$   
(at  $P=10\text{MPa}$ ,  $T=40^\circ\text{C}$ )
- Injection rate:  
 $1 \text{ Mt/year/hole} \times 10 \text{ holes}$   
 $= 10 \text{ Mt/year}$
- Assume CO<sub>2</sub> injection over a period of 100 years.
- Simulation is performed until 1000 years

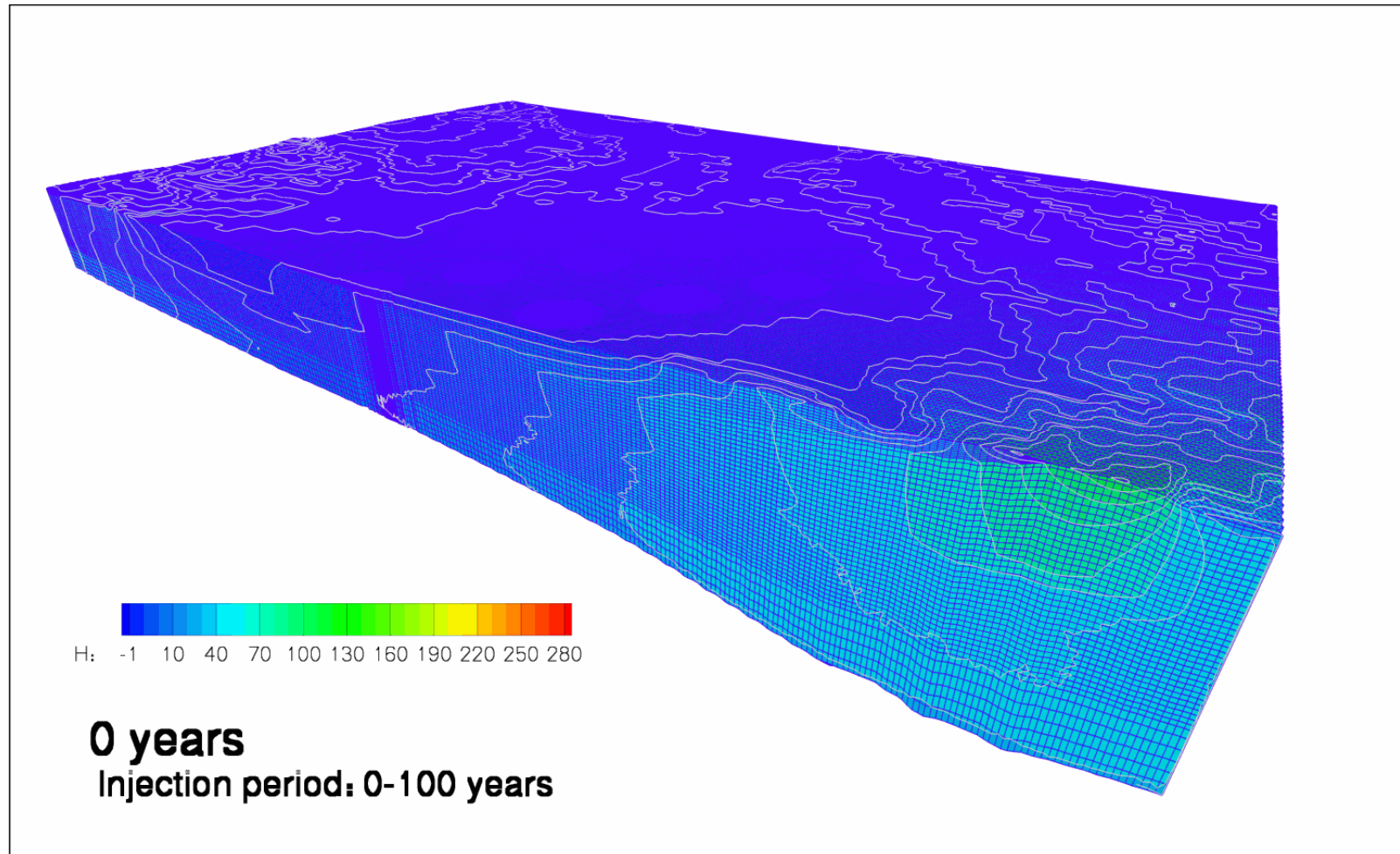


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# Results –CO<sub>2</sub> migration-



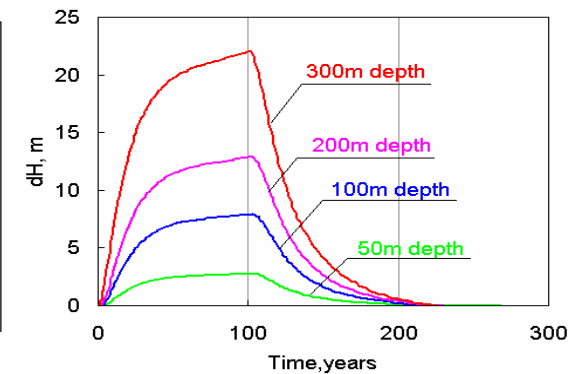
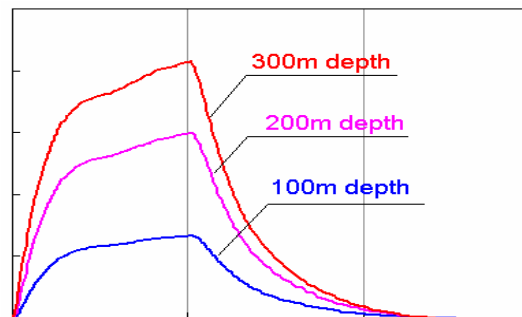
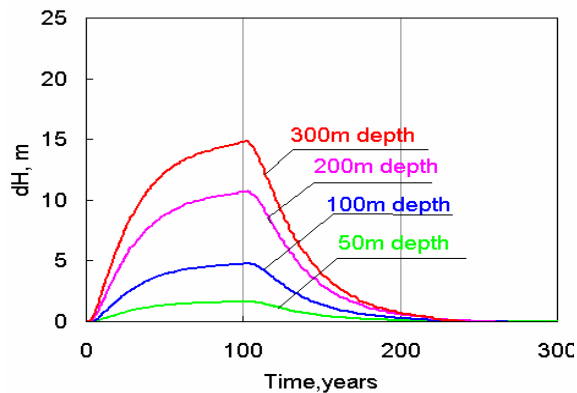
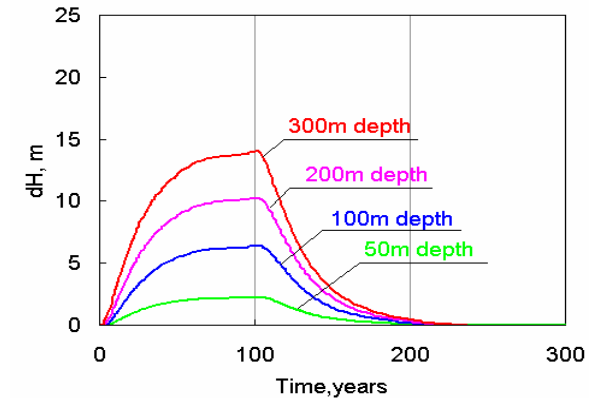
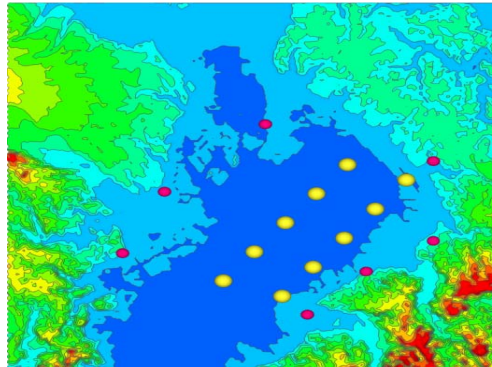
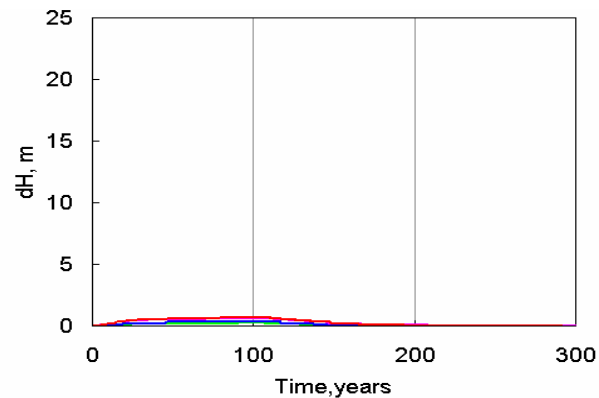
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# Results –Head Build-up (1)- Change in head with time at urban inlands



Base Case (Continuous Layer Model)

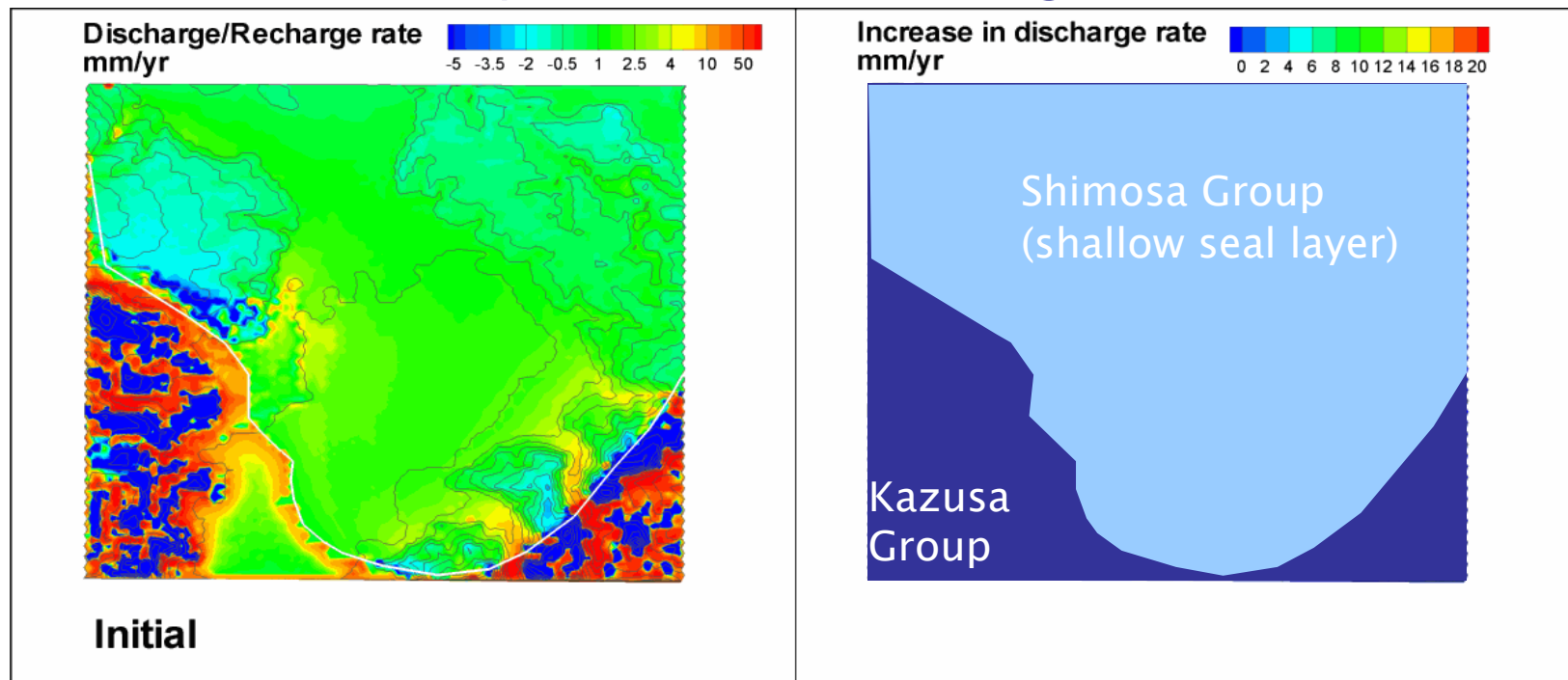
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# Results –Surface Discharge –

How much water pushed out is discharged at the surface



Base Case

Discharge occurs in the sea floor and under the boundary of Shimosa/Kazusa G.

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## Example 2: Dissolution-Diffusion-Convection Process( Zhang and Pruess 2007)

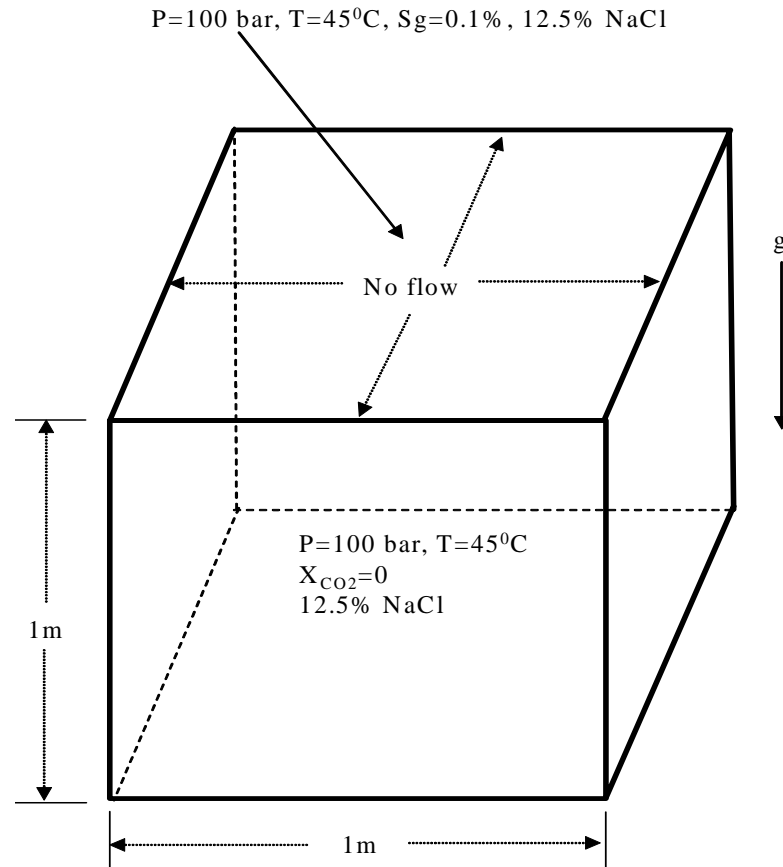
- ✓ Role of irregular features (geometry, heterogeneity) and 3-Deffects in “real” systems?
- ✓ Growth of dissolved CO<sub>2</sub> inventory.
- ✓ How can the multi-scale nature of the dissolution-diffusion-convection process be captured in field-scale simulations?



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# 3D Model



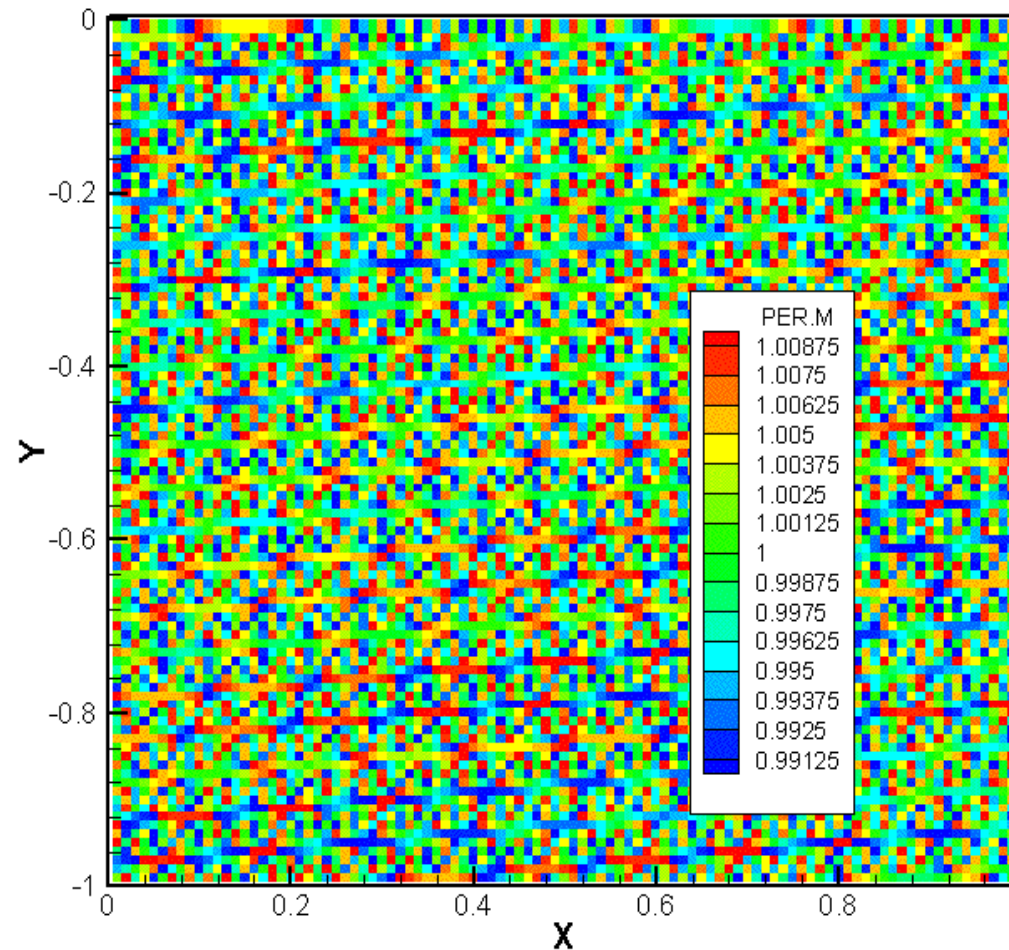
3-D domain for  
simulating brine  
convection induced by  
CO<sub>2</sub> dissolution and  
associated increase in  
aqueous phase density.  
(X<sub>co2</sub>=0.0493 at top  
boundary)



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# Random Heterogeneity Field for Triggering Brine Convection



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# Characterizing DDC Processes

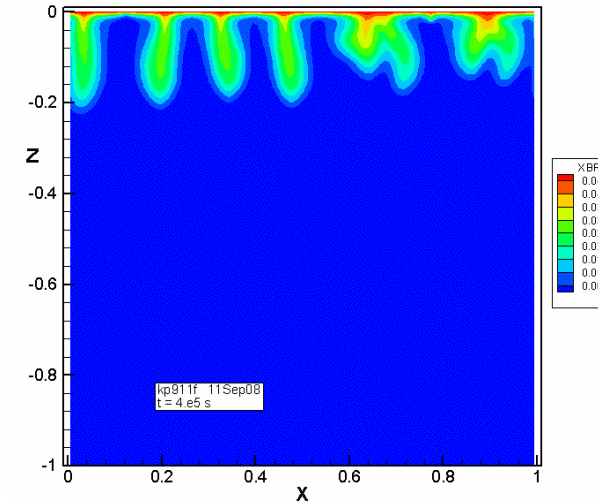
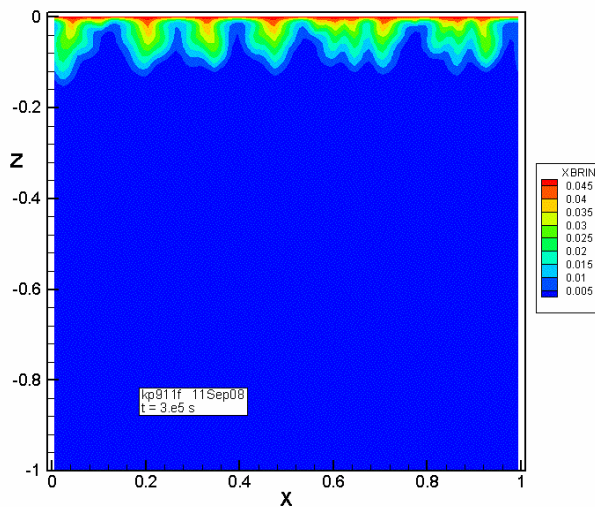
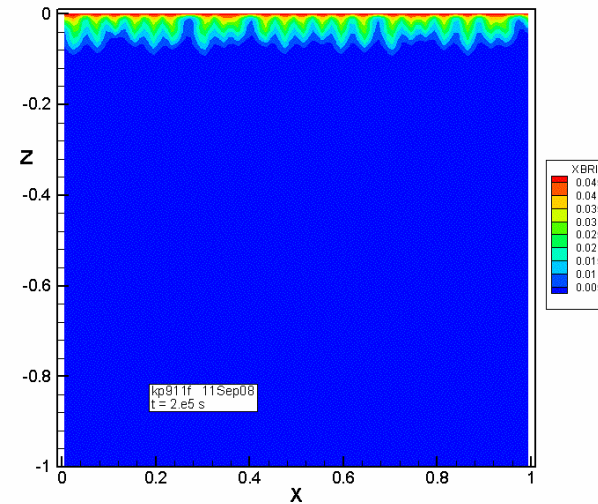
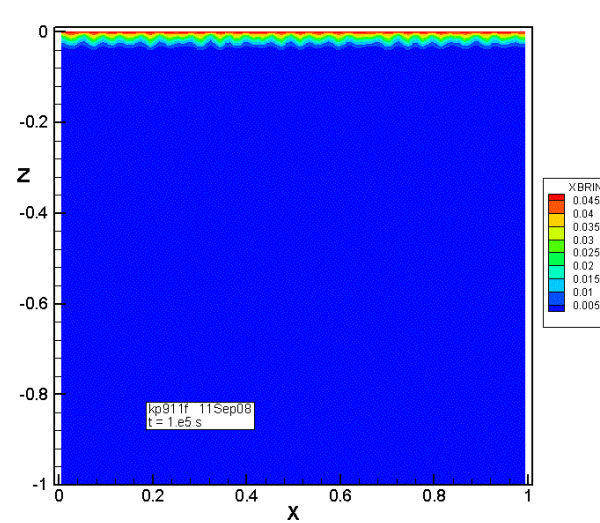
- ✓ Constant dissolved concentration at the interface
- ✓ The rate of CO<sub>2</sub> entering the system equals to its dissolution rate at the top boundary.
- ✓ The growth of total dissolved CO<sub>2</sub> inventory over time
- ✓ Comparison with the case without convection
- ✓ Investigating different random seeds



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# Dissolved CO<sub>2</sub> concentrations at different times

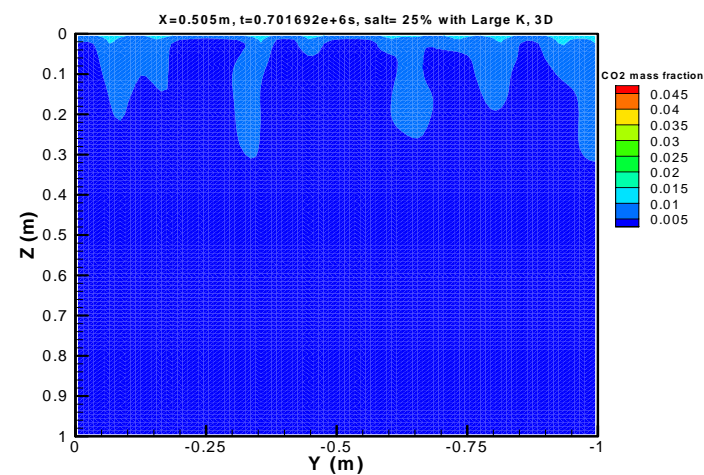
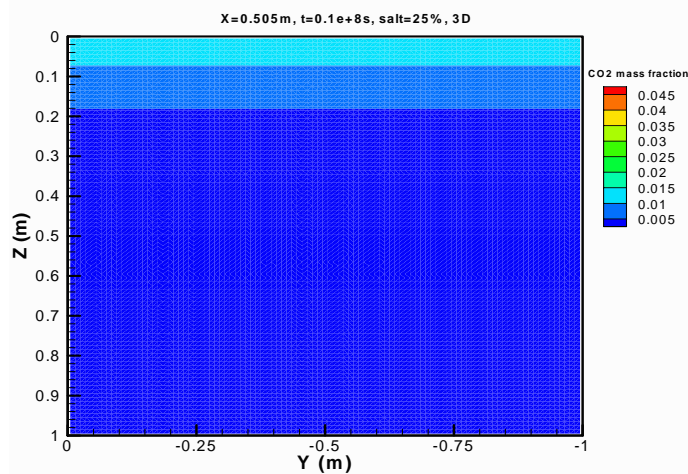
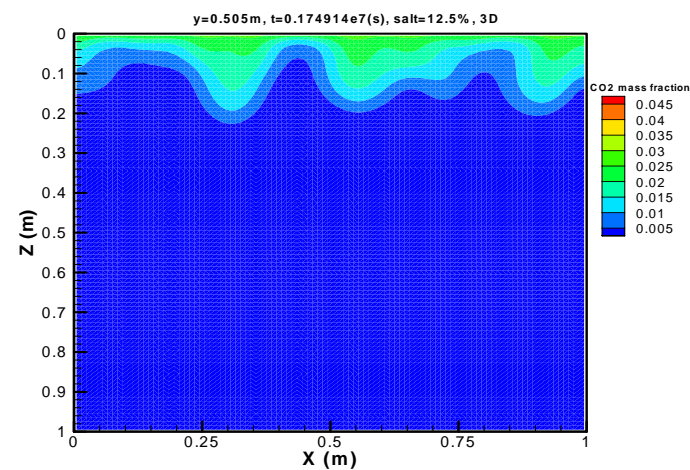
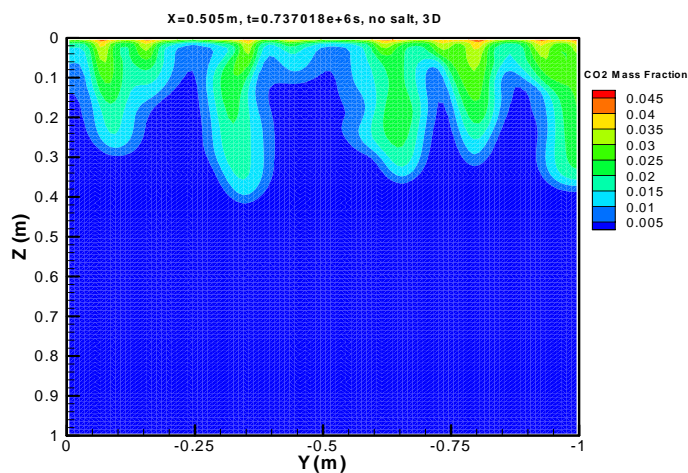


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# 3D Model results



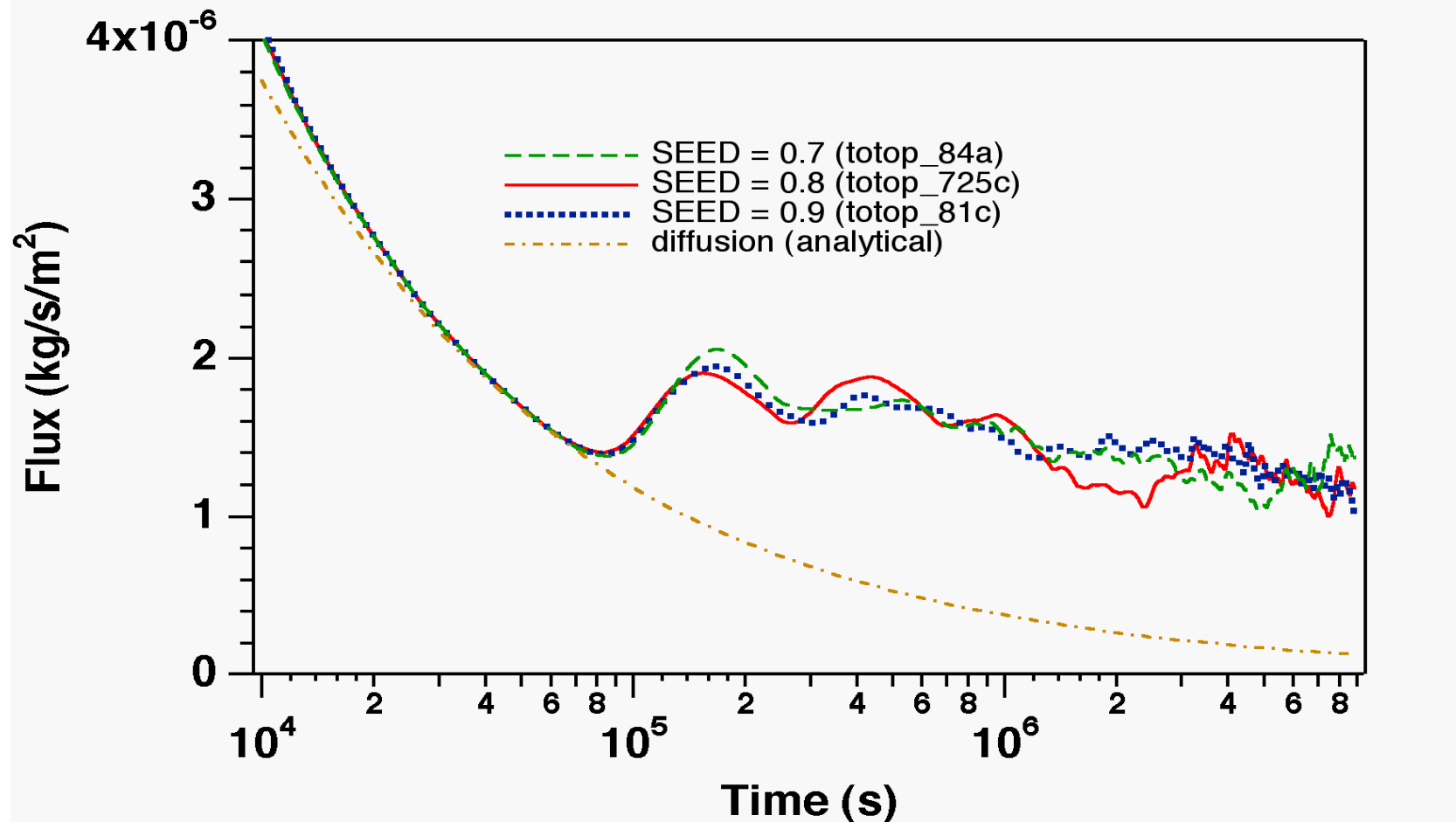
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# Random permeability influence on CO<sub>2</sub> flux at top boundary



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# Thank you



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